APPENDIX 1

The surface science of titanium dioxide

Ulrike Diebold[*]

Department of Physics, Tulane University, New Orleans, LA 70118, USA

Manuscript received in final form 7 October 2002

2.5. Vicinal and other rutile surfaces

Vicinal surfaces of TiO₂ have not been studied extensively. A study of Na adsorption on a stepped (4 4 1) surface was reported by Onishi et al. [205]. Unpublished experiments from this author's laboratory with a similarly cut crystal showed macroscopic faceting upon annealing.

The most detailed investigation was performed recently on a $TiO_2(2\ 1\ 0)$ surface [206]. In a formal sense, $TiO_2(2\ 1\ 0)$ lies midways between (1 1 0) and (1 0 0), and is the most simple vicinal surface. Atomistic simulations, based on Coulombic interaction between ions and a short-range repulsive interaction, predicted an asymmetric sawtooth-like structure of the surface, consisting of {1 1 0} nanofacets. The width of each nanofacet is 1.5 times the width of the surface unit cell of the (1 1 0)-(1 × 1) structure (i.e. $3a/\sqrt{2}$). The nanofacets terminate with a row of Ti atoms carrying bridging oxygen atoms. The surface energy of this structure is predicted to be $2.07\ J/m^2$. (This is to be compared to a surface energy of $1.78\ J/m^2$ derived using a similar calculation for $TiO_2(1\ 1\ 0)$ [206].) STM images showed a (1 × 1)-terminated surface that could be consistent with this structure, although the interpretation was again made difficult by balancing electronic effects with the very strong corrugations of this surface.

The structure of the $TiO_2(1\ 1\ 1)$ surface was investigated by Onishi and co-workers [207] with LEED and STM. Depending on the annealing temperature, the surface shows a variety of reconstructions.

4.1.2. Growth morphology (thermodynamic equilibrium)

It is useful (though a quite rough oversimplification, see below) to distinguish three film growth modes in thermodynamic equilibrium. When the difference between the surface free energy of the clean substrate, $\gamma_{substrate}$, and surface free energy of the overlayer metal, γ_{metal}, is greater than the interfacial energy, $\gamma_{interface}$, i.e.,

$$\gamma_{interface} > \gamma_{substrate} - \gamma_{metal} \tag{4}$$

cluster growth (also called Volmer–Weber growth) should take place. When it is less, the film should wet. For thicker films, growth can proceed in a layer-by-layer fashion (Frank–van der Merwe growth mode). Often, epitaxial strain increases in thicker films and breaks up the overlayer (layer + clusters or Stranski–Krastanov growth mode). Because the surface energy of virtually all clean metals is higher than that of TiO₂ (where an experimental value of $\sim0.35\ J/m^2$ was reported [291]) the term on the left side is negative. Hence, cluster growth should occur, unless $\gamma_{interface}$ itself has a *negative* value. It has been suggested [10,63,292] that this is the case for very reactive overlayers, where an interfacial reaction as in Eqs. (1)–(3) is thermodynamically favored.

APPENDIX 2

Polymeerien pintajännityksiä kirjasta POLYMER HANDBOOK
(Wiley)

	20 C mN/m = dyn/cm
PTFE	23,9
PA11 (225 C)	22,6
TPX	25
PP, isotactic	29,4
EVA 82/18	34,1
PE (LD, Mn7000)	35,3
PA12	35,8
PA6	38,4
PS (Mn9300)	39,4
PMMA (M=3000)	41,1
PVC	41,9
PC (sulasta)	42,9
SAN (33% acrylon.)	43
PET (Mn16000)	44,6
POM (homopolym.)	44,6
PC	45
PA66	46,5
PBT(isophalate)	47,8
(acrylonit.-butadien, 3:7)	52,6

APPENDIX 3

Tällainen tieto löytyi:

Interfacial interaction and mechanical properties of nylon 6-potassium titanate composites prepared by in-situ polymerization

Ou Yuchun*, Yang Feng, Chen Jin

State Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100080, People's Republic of China

Abstract

A new method was proposed for the synthesis of nylon 6-potassium titanate composites with high strength and high modulus. Dispersion quality of potassium titanate whiskers in the polyamide matrix and the degree of interfacial adhesion between polyamide and whiskers are the key points with ε-caproamide and potassium titanate whiskers, which were modified by an alkylsilane coupling agent with n-aminocapric acid as initiator through *in-situ* polymerization. The contact angle test showed that the **surface energy of modified whiskers is similar to nylon 6's, while that of the unmodified ones was much higher than nylon 6's**. These results suggest that the modified whiskers would disperse homogeneously in the nylon 6 matrix. Scanning electronic microscope (SEM) results fortified the above hypothesis. According to infrared (IR) spectra, the sample of whiskers that were separated from the modified composite by formic acid have the characteristic peak of nylon 6's; and the whiskers that were separated from unmodified composite do not have them, which suggested that there are chemical bonds between modified whiskers and nylon 6 matrix, and the whiskers served as chemical cross-link points in the composite. © 1997 John Wiley & Sons, Inc. J Appl Polym Sci 64: 2317-2322, 1997

*Correspondence to Ou Yuchun, State Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100080, People's Republic of Chin